

N-(2-((1-(Cyclohexylmethyl)-2-(3-ethyl-2-oxo-5-oxazolidinyl)-2-hydroxyethyl)amino)-2-oxo-1-(2-thienylmethyl)ethyl)-gamma-oxo-alpha-(phenylmethyl)-4-morpholinebutanamide  
122225-00-7 | DTXSID80153548

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 9.61

Global applicability domain: Outside

Local applicability domain index: 1.19e-01

Confidence level: 4.53e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Hydroxybenzoic acid</div> <div>Measured: 8.08</div> <div>Predicted: 7.78</div>	<div>Image not found</div> <div>Salicylic acid</div> <div>Measured: 7.44</div> <div>Predicted: 7.60</div>	<div>Image not found</div> <div>1-Eicosanol</div> <div>Measured: 12.1</div> <div>Predicted: 11.2</div>
<div>Image not found</div> <div>1-Octadecanol</div> <div>Measured: 10.9</div> <div>Predicted: 10.5</div>	<div>Image not found</div> <div>1-Hexadecanol</div> <div>Measured: 9.90</div> <div>Predicted: 9.79</div>	